



wwPDB EM Validation Summary Report ⓘ

Jul 3, 2023 – 12:37 PM JST

PDB ID : 8IUH
EMDB ID : EMD-35722
Title : RNA polymerase III pre-initiation complex open complex 1
Authors : Hou, H.; Jin, Q.; Ren, Y.; Wang, Q.; Xu, Y.
Deposited on : 2023-03-24
Resolution : 3.40 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev50
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.34

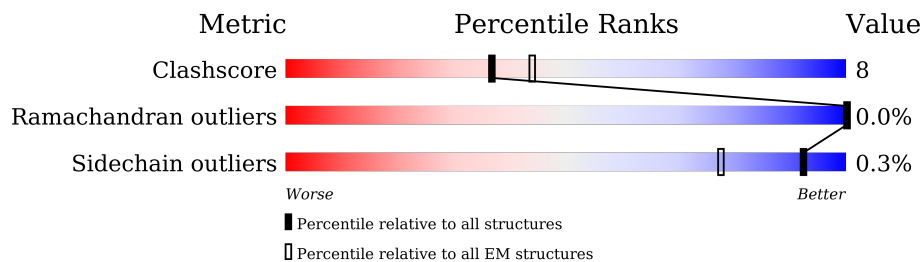
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	368	
2	3	411	
3	4	1469	
4	A	1390	
5	B	1133	
6	C	346	
7	D	148	
8	E	210	

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Mol	Chain	Length	Quality of chain
9	F	127	54% 6% 40%
10	G	204	60% 21% 19%
11	H	150	79% 19%
12	I	108	22% 74% 25%
13	J	67	76% 21%
14	K	133	68% 9% 23%
15	L	58	55% 24% 21%
16	M	708	5% 50% 9% 40%
17	N	317	36% 10% 54%
18	O	534	7% 84% 12%
19	P	316	18% 79% 16%
20	Q	223	34% 5% 61%
21	U	339	46% 6% 48%
22	V	419	7% 72% 14% 14%
23	W	2624	96%
24	X	464	6% 12% 83%
25	Y	464	8% 10% 83%

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 58239 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called snRNA-activating protein complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	146	1233	804	212	209	8	0	0

- Molecule 2 is a protein called snRNA-activating protein complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	374	3037	1925	521	570	21	0	0

- Molecule 3 is a protein called snRNA-activating protein complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	365	3058	1921	573	555	9	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	1378	10814	6850	1886	2005	73	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	1097	8680	5499	1516	1597	68	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	343	2736	1723	488	514	11	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D	122	985	614	172	196	3	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	E	209	1715	1083	300	324	8	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	F	76	610	392	103	110	5	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	G	166	1337	876	211	245	5	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	H	148	1186	750	194	237	5	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	I	107	848	525	157	153	13	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	24	ALA	SER	variant	UNP Q9Y2Y1

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	65	Total	C	N	O	S	0	0
			512	331	87	88	6		

- Molecule 14 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	103	Total	C	N	O	S	0	0
			822	513	145	157	7		

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	422	Total	C	N	O	S	0	0
			3382	2138	588	636	20		

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	146	Total	C	N	O	S	0	0
			1128	710	191	221	6		

There are 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	LYS	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	PHE	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	GLY	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	ARG	deletion	UNP P05423
N	?	-	ASN	deletion	UNP P05423

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Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	ASP	deletion	UNP P05423
N	?	-	THR	deletion	UNP P05423
N	?	-	ARG	deletion	UNP P05423
N	?	-	ASN	deletion	UNP P05423
N	?	-	MET	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	VAL	deletion	UNP P05423
N	?	-	GLN	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	HIS	deletion	UNP P05423
N	?	-	SER	deletion	UNP P05423
N	?	-	GLY	deletion	UNP P05423
N	?	-	TRP	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	PHE	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	ASN	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	VAL	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	TRP	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	GLY	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	MET	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	VAL	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423

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Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	ILE	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	VAL	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	VAL	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	ARG	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	MET	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	ARG	deletion	UNP P05423

- Molecule 18 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	O	512	4075	2565	712	774	24	0	0

- Molecule 19 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	P	303	2403	1516	411	460	16	0	0

- Molecule 20 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	87	Total	C	N	O	S	0	0
			754	488	126	134	6		

- Molecule 21 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	176	Total	C	N	O	S	1	0
			1396	907	244	238	7		

- Molecule 22 is a protein called Transcription factor IIIB 50 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	361	Total	C	N	O	S	1	0
			2853	1792	507	531	23		

- Molecule 23 is a protein called Transcription factor TFIIB component B' homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	111	Total	C	N	O	S	0	0
			943	606	163	170	4		

- Molecule 24 is a DNA chain called DNA (81-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	81	Total	C	N	O	P	0	0
			1661	795	288	497	81		

- Molecule 25 is a DNA chain called DNA (81-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	81	Total	C	N	O	P	0	0
			1666	793	317	475	81		

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
26	A	2	Total	Zn	0
			2	2	
26	B	1	Total	Zn	0
			1	1	
26	I	2	Total	Zn	0
			2	2	

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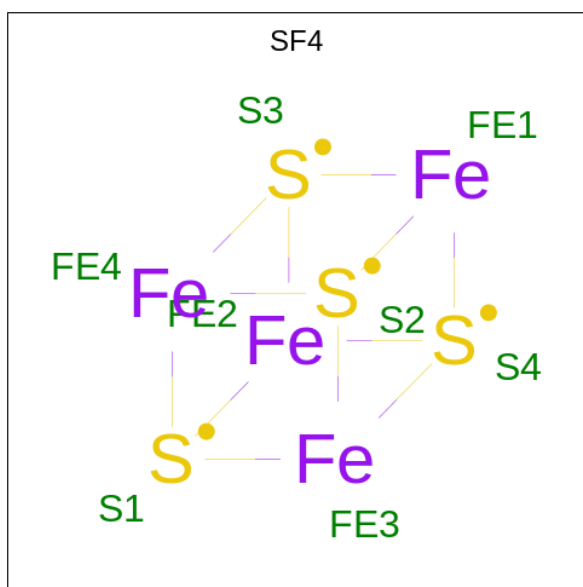
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Mol	Chain	Residues	Atoms		AltConf
26	J	1	Total	Zn	0
			1	1	
26	L	1	Total	Zn	0
			1	1	
26	V	1	Total	Zn	0
			1	1	

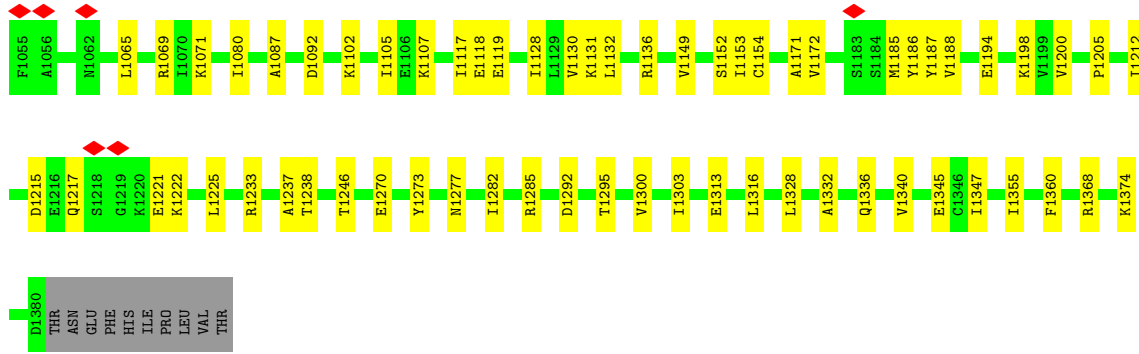
- Molecule 27 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
27	A	1	Total	Mg	0
			1	1	

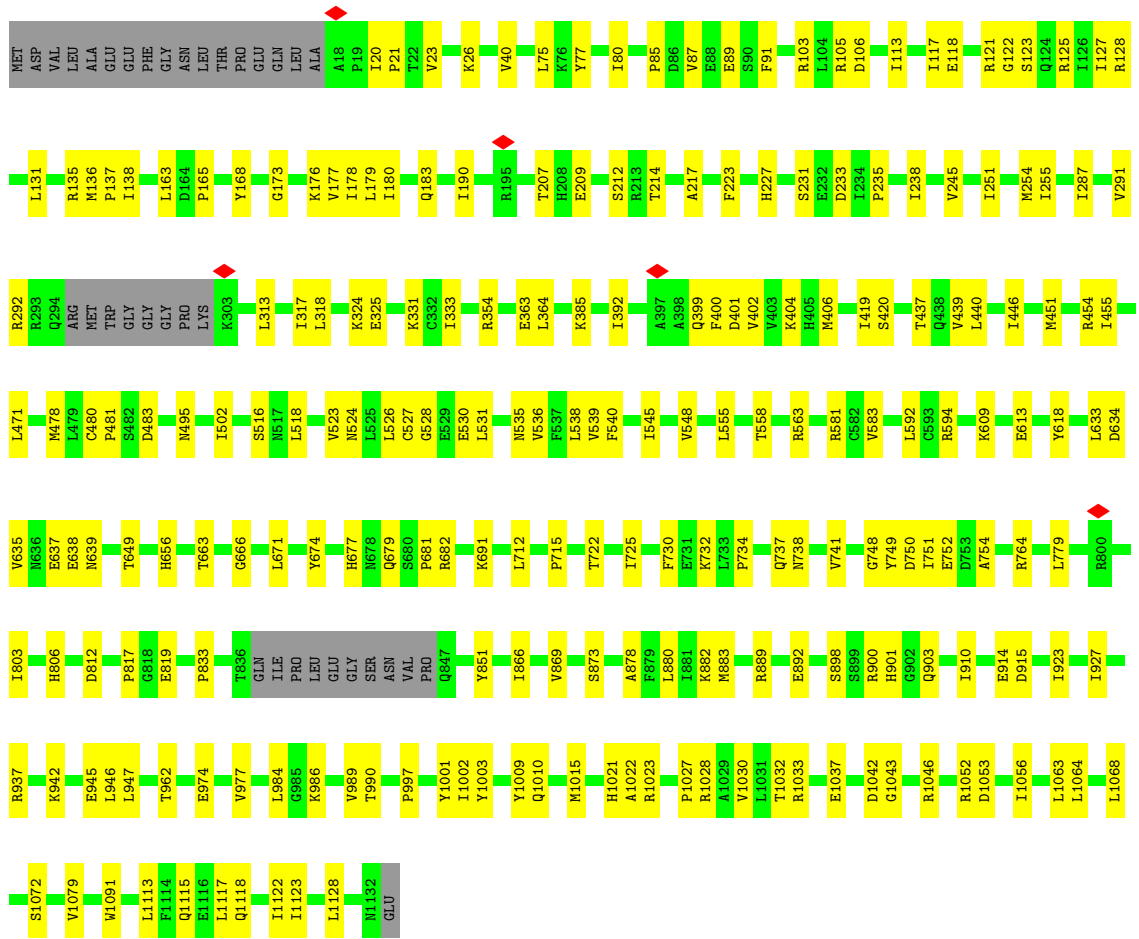
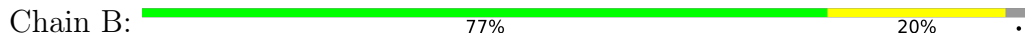
- Molecule 28 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



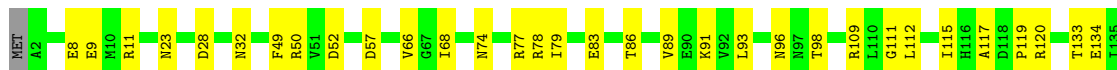
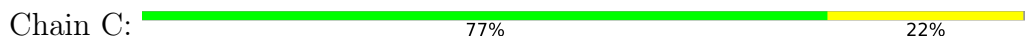
Mol	Chain	Residues	Atoms			AltConf
28	P	1	Total	Fe	S	0
			8	4	4	

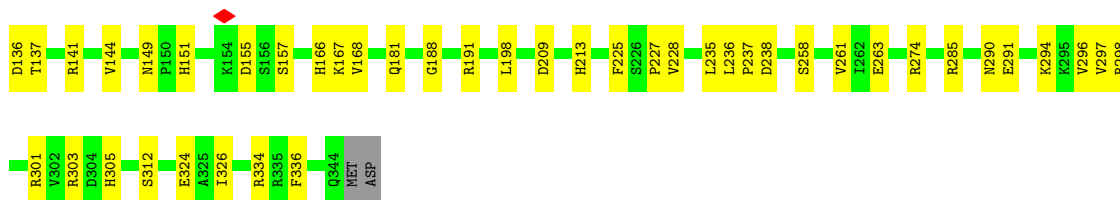


• Molecule 5: DNA-directed RNA polymerase III subunit RPC2

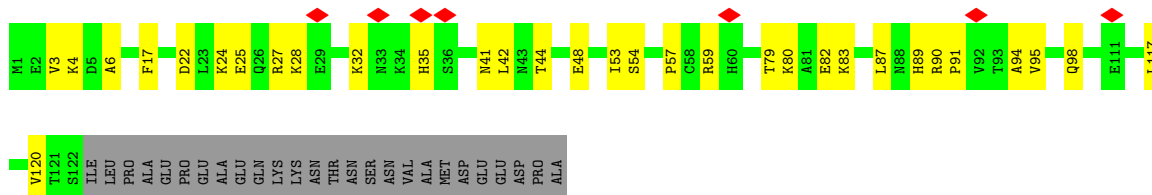


• Molecule 6: DNA-directed RNA polymerases I and III subunit RPAC1

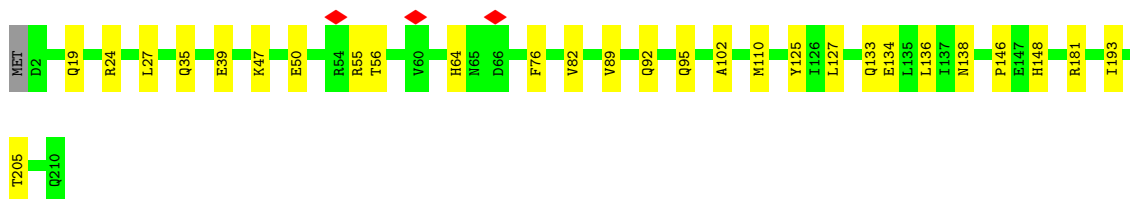
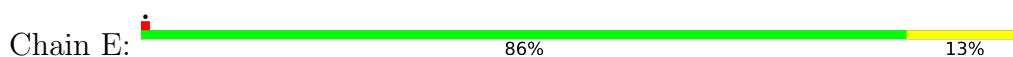




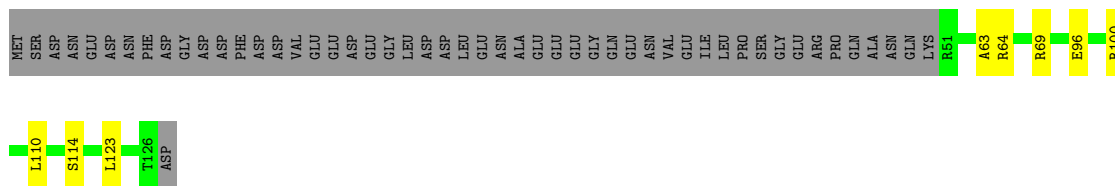
- Molecule 7: DNA-directed RNA polymerase III subunit RPC9



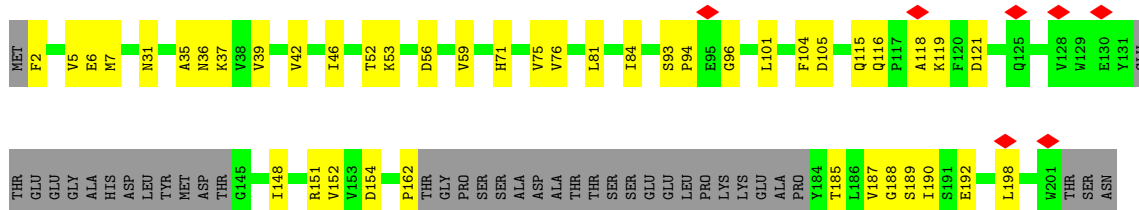
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC1



- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC2



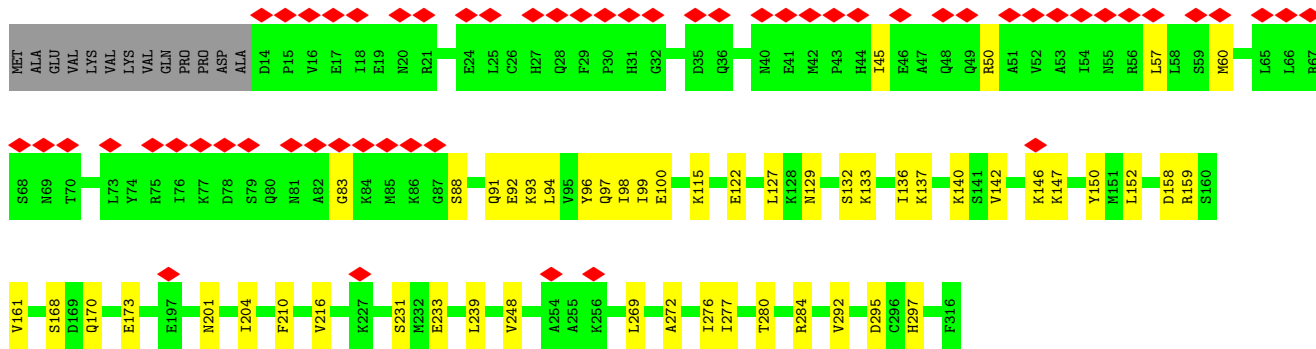
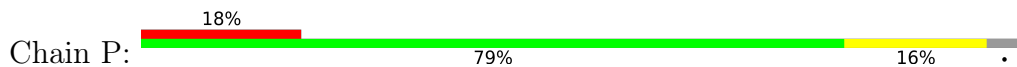
- Molecule 10: DNA-directed RNA polymerase III subunit RPC8



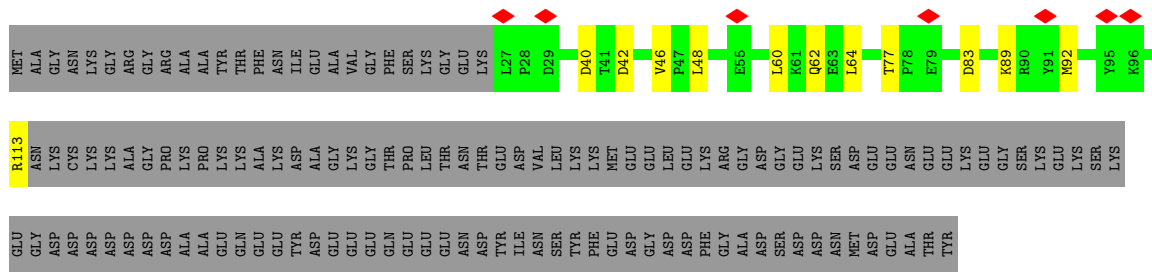
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC3



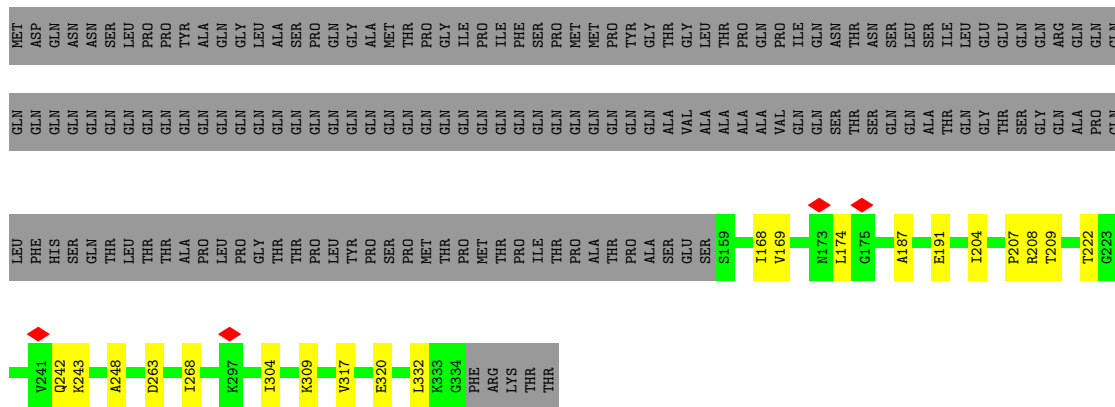
• Molecule 19: DNA-directed RNA polymerase III subunit RPC6



• Molecule 20: DNA-directed RNA polymerase III subunit RPC7



• Molecule 21: TATA-box-binding protein



• Molecule 22: Transcription factor IIIB 50 kDa subunit

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	107630	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.271	Depositor
Minimum map value	-0.107	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	426.88, 426.88, 426.88	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.334, 1.334, 1.334	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SF4, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.24	0/1266	0.38	0/1708
2	3	0.24	0/3112	0.41	0/4206
3	4	0.23	0/3121	0.38	0/4181
4	A	0.24	0/11008	0.40	0/14842
5	B	0.24	0/8845	0.40	0/11930
6	C	0.23	0/2790	0.40	0/3782
7	D	0.23	0/997	0.39	0/1343
8	E	0.23	0/1745	0.39	0/2358
9	F	0.22	0/620	0.38	0/839
10	G	0.24	0/1374	0.42	0/1868
11	H	0.24	0/1207	0.42	0/1628
12	I	0.23	0/869	0.42	0/1174
13	J	0.23	0/521	0.36	0/703
14	K	0.23	0/837	0.41	0/1129
15	L	0.23	0/394	0.42	0/524
16	M	0.23	0/3455	0.38	0/4673
17	N	0.23	0/1137	0.44	0/1530
18	O	0.23	0/4141	0.39	0/5592
19	P	0.23	0/2446	0.36	0/3301
20	Q	0.23	0/777	0.38	0/1050
21	U	0.24	0/1424	0.43	0/1918
22	V	0.23	0/2904	0.39	0/3941
23	W	0.24	0/967	0.38	0/1293
24	X	0.52	0/1858	0.96	0/2865
25	Y	0.48	0/1872	0.86	0/2884
All	All	0.26	0/59687	0.45	0/81262

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1233	0	1231	46	0
2	3	3037	0	2911	75	0
3	4	3058	0	3064	56	0
4	A	10814	0	11057	215	0
5	B	8680	0	8805	179	0
6	C	2736	0	2712	55	0
7	D	985	0	1006	24	0
8	E	1715	0	1733	20	0
9	F	610	0	642	5	0
10	G	1337	0	1306	34	0
11	H	1186	0	1147	18	0
12	I	848	0	809	20	0
13	J	512	0	525	14	0
14	K	822	0	810	11	0
15	L	388	0	394	10	0
16	M	3382	0	3376	52	0
17	N	1128	0	1181	26	0
18	O	4075	0	4149	43	0
19	P	2403	0	2409	42	0
20	Q	754	0	759	13	0
21	U	1396	0	1490	18	0
22	V	2853	0	2892	71	0
23	W	943	0	924	16	0
24	X	1661	0	922	61	0
25	Y	1666	0	911	32	0
26	A	2	0	0	0	0
26	B	1	0	0	0	0
26	I	2	0	0	0	0
26	J	1	0	0	0	0
26	L	1	0	0	0	0
26	V	1	0	0	0	0
27	A	1	0	0	0	0
28	P	8	0	0	0	0
All	All	58239	0	57165	949	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 949 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:191:ILE:HB	3:4:176:PHE:CZ	1.59	1.36
22:V:111:LEU:HD13	24:X:-17:DT:OP2	1.24	1.30
1:1:63:TRP:HE3	1:1:82:LEU:CD1	1.51	1.24
5:B:113:ILE:HD11	5:B:136:MET:CB	1.73	1.17
2:3:101:ARG:HA	2:3:104:CYS:SG	1.83	1.16

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	144/368 (39%)	142 (99%)	2 (1%)	0	100	100
2	3	368/411 (90%)	352 (96%)	15 (4%)	1 (0%)	41	72
3	4	363/1469 (25%)	353 (97%)	10 (3%)	0	100	100
4	A	1376/1390 (99%)	1350 (98%)	26 (2%)	0	100	100
5	B	1091/1133 (96%)	1062 (97%)	29 (3%)	0	100	100
6	C	341/346 (99%)	336 (98%)	5 (2%)	0	100	100
7	D	120/148 (81%)	115 (96%)	5 (4%)	0	100	100
8	E	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
9	F	74/127 (58%)	72 (97%)	2 (3%)	0	100	100
10	G	160/204 (78%)	144 (90%)	16 (10%)	0	100	100
11	H	146/150 (97%)	145 (99%)	1 (1%)	0	100	100
12	I	105/108 (97%)	98 (93%)	7 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	J	63/67 (94%)	62 (98%)	1 (2%)	0	100	100
14	K	101/133 (76%)	97 (96%)	4 (4%)	0	100	100
15	L	44/58 (76%)	42 (96%)	2 (4%)	0	100	100
16	M	418/708 (59%)	405 (97%)	13 (3%)	0	100	100
17	N	140/317 (44%)	139 (99%)	1 (1%)	0	100	100
18	O	508/534 (95%)	497 (98%)	11 (2%)	0	100	100
19	P	301/316 (95%)	296 (98%)	5 (2%)	0	100	100
20	Q	85/223 (38%)	84 (99%)	1 (1%)	0	100	100
21	U	175/339 (52%)	171 (98%)	4 (2%)	0	100	100
22	V	358/419 (85%)	352 (98%)	6 (2%)	0	100	100
23	W	109/2624 (4%)	105 (96%)	4 (4%)	0	100	100
All	All	6797/11802 (58%)	6622 (97%)	174 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	3	341	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	130/334 (39%)	130 (100%)	0	100	100
2	3	330/356 (93%)	323 (98%)	7 (2%)	53	76
3	4	321/1213 (26%)	318 (99%)	3 (1%)	78	90
4	A	1200/1212 (99%)	1197 (100%)	3 (0%)	92	97
5	B	959/988 (97%)	959 (100%)	0	100	100
6	C	299/302 (99%)	299 (100%)	0	100	100
7	D	114/136 (84%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	E	191/192 (100%)	191 (100%)	0	100	100
9	F	66/111 (60%)	66 (100%)	0	100	100
10	G	149/181 (82%)	149 (100%)	0	100	100
11	H	129/131 (98%)	129 (100%)	0	100	100
12	I	92/93 (99%)	92 (100%)	0	100	100
13	J	53/56 (95%)	53 (100%)	0	100	100
14	K	92/119 (77%)	92 (100%)	0	100	100
15	L	43/55 (78%)	43 (100%)	0	100	100
16	M	377/622 (61%)	377 (100%)	0	100	100
17	N	131/276 (48%)	130 (99%)	1 (1%)	81	91
18	O	458/476 (96%)	457 (100%)	1 (0%)	93	98
19	P	269/280 (96%)	268 (100%)	1 (0%)	91	95
20	Q	84/195 (43%)	83 (99%)	1 (1%)	71	85
21	U	152/293 (52%)	152 (100%)	0	100	100
22	V	325/365 (89%)	323 (99%)	2 (1%)	86	94
23	W	102/2381 (4%)	101 (99%)	1 (1%)	76	88
All	All	6066/10367 (58%)	6046 (100%)	20 (0%)	92	97

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	O	533	ARG
22	V	55	TYR
23	W	309	ASP
22	V	381	ASP
2	3	386	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
6	C	160	ASN
23	W	327	GLN
16	M	11	GLN
23	W	279	ASN
21	U	278	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
28	SF4	P	401	-	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SF4	P	401	-	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

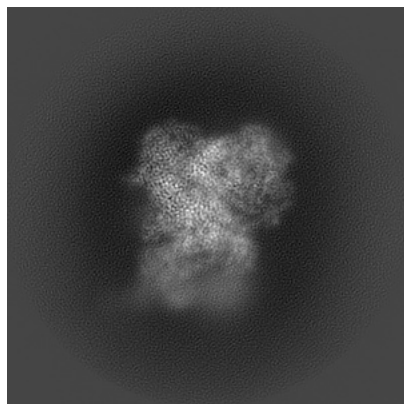
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35722. These allow visual inspection of the internal detail of the map and identification of artifacts.

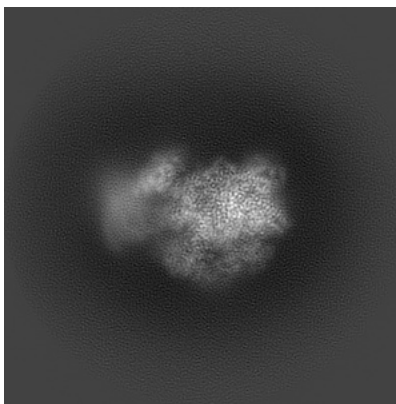
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

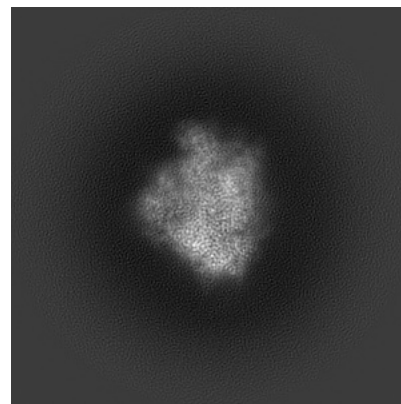
6.1.1 Primary map



X

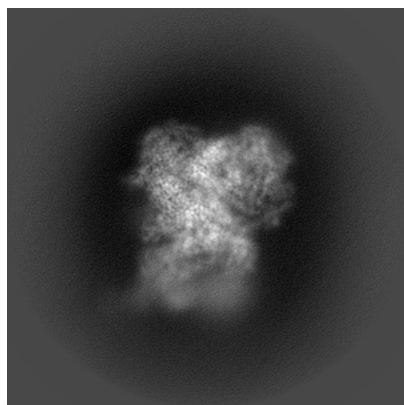


Y

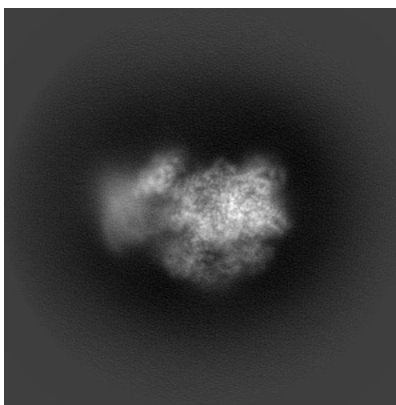


Z

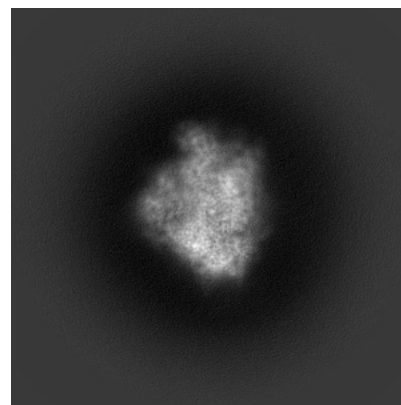
6.1.2 Raw map



X



Y

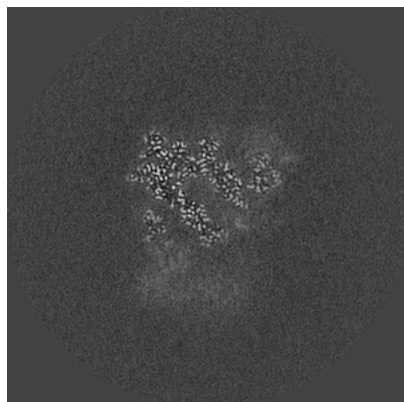


Z

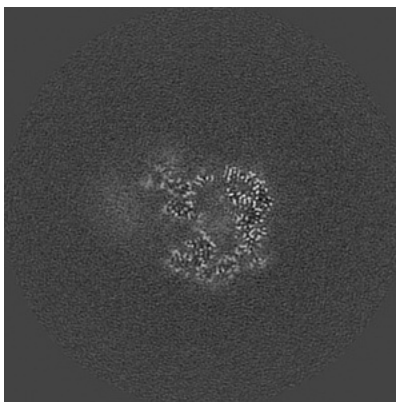
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

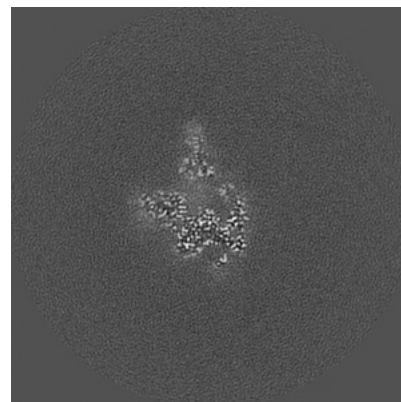
6.2.1 Primary map



X Index: 160

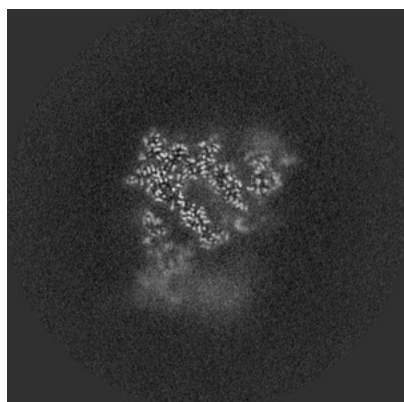


Y Index: 160

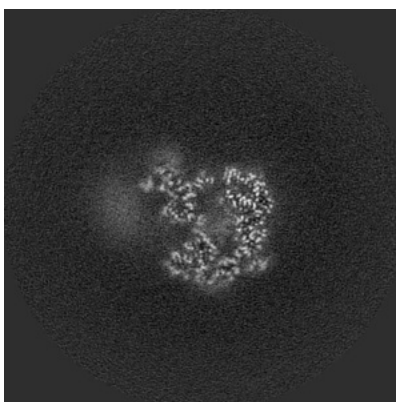


Z Index: 160

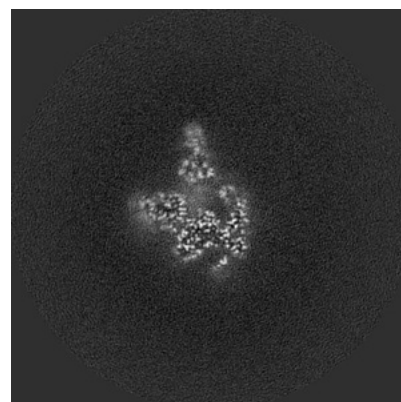
6.2.2 Raw map



X Index: 160



Y Index: 160

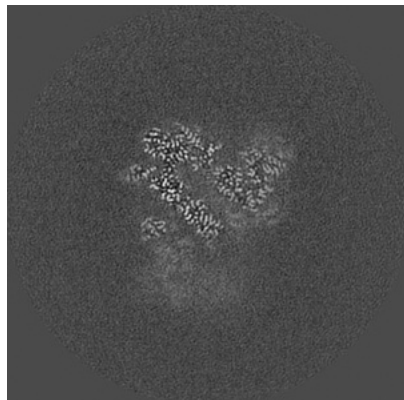


Z Index: 160

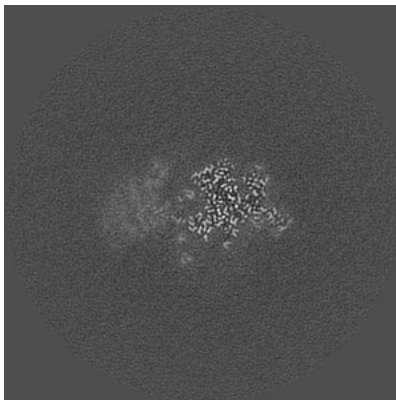
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

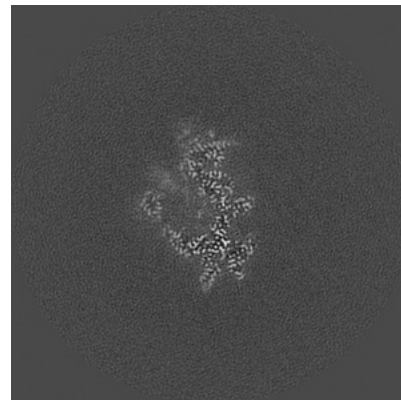
6.3.1 Primary map



X Index: 155

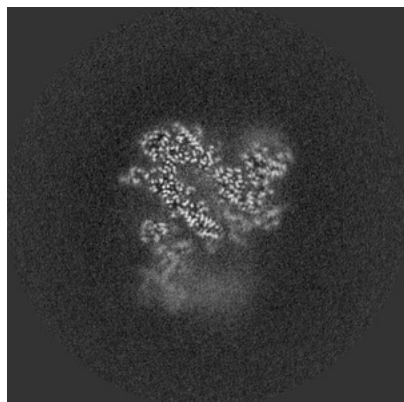


Y Index: 129

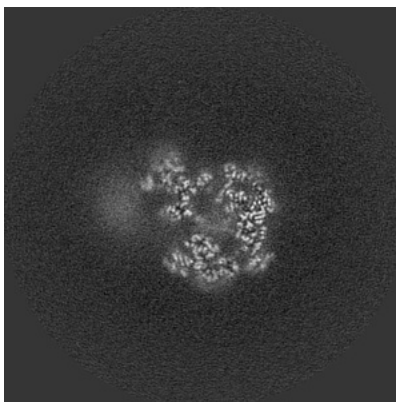


Z Index: 181

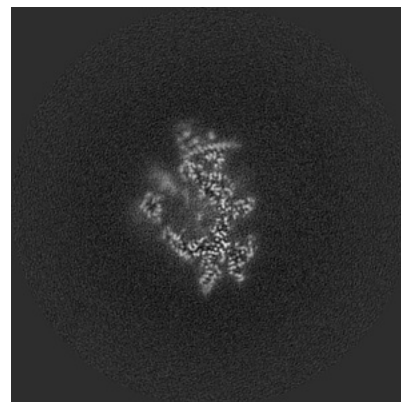
6.3.2 Raw map



X Index: 154



Y Index: 162

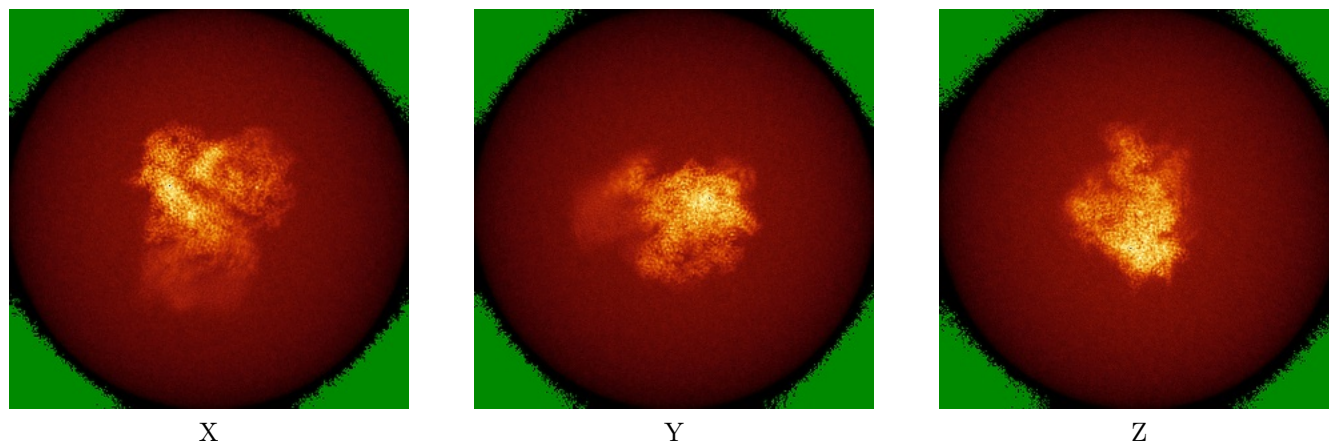


Z Index: 181

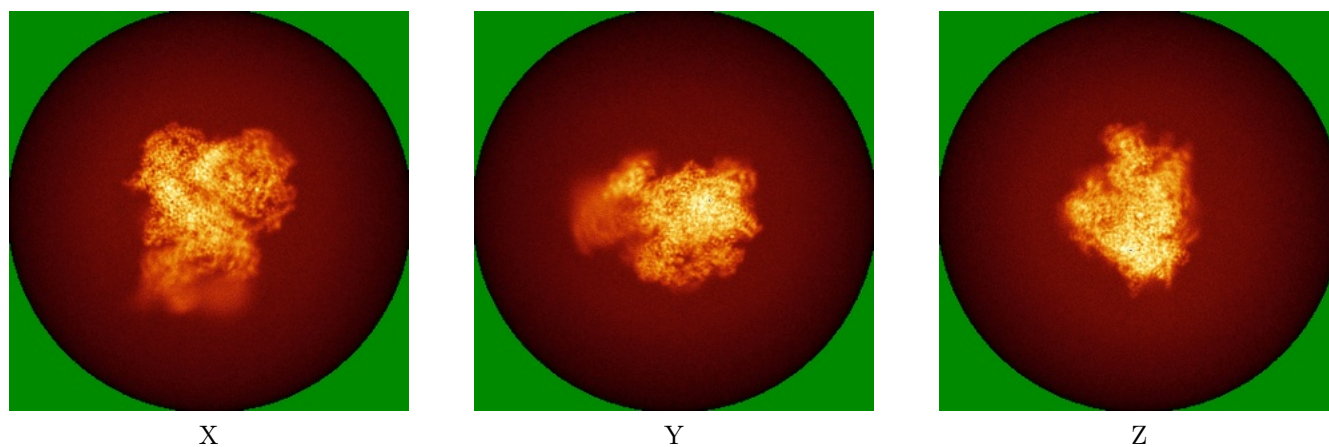
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



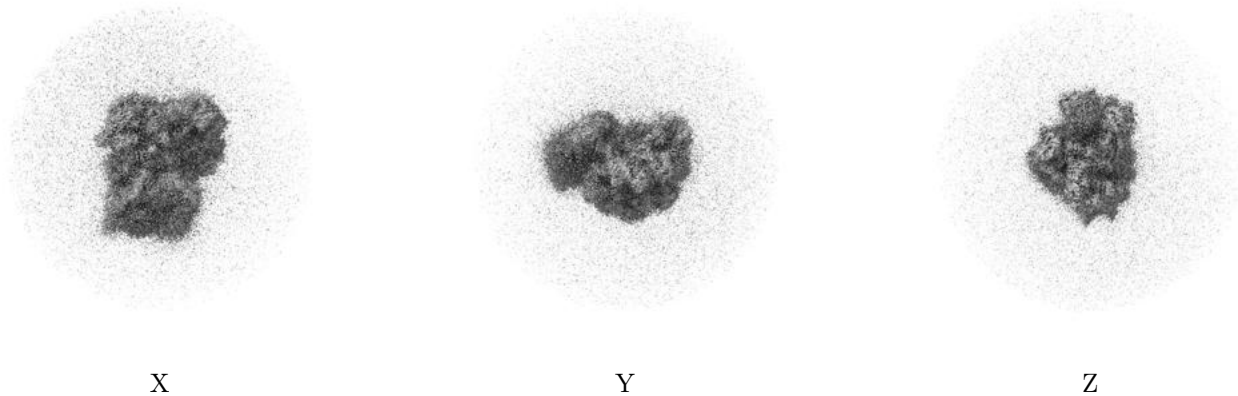
6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

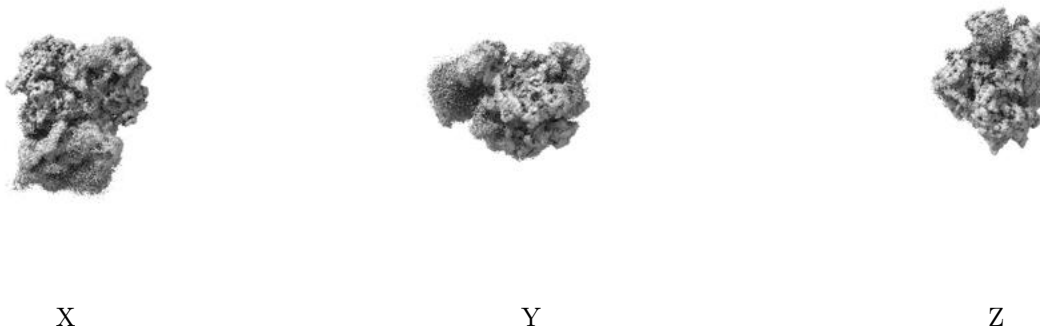
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

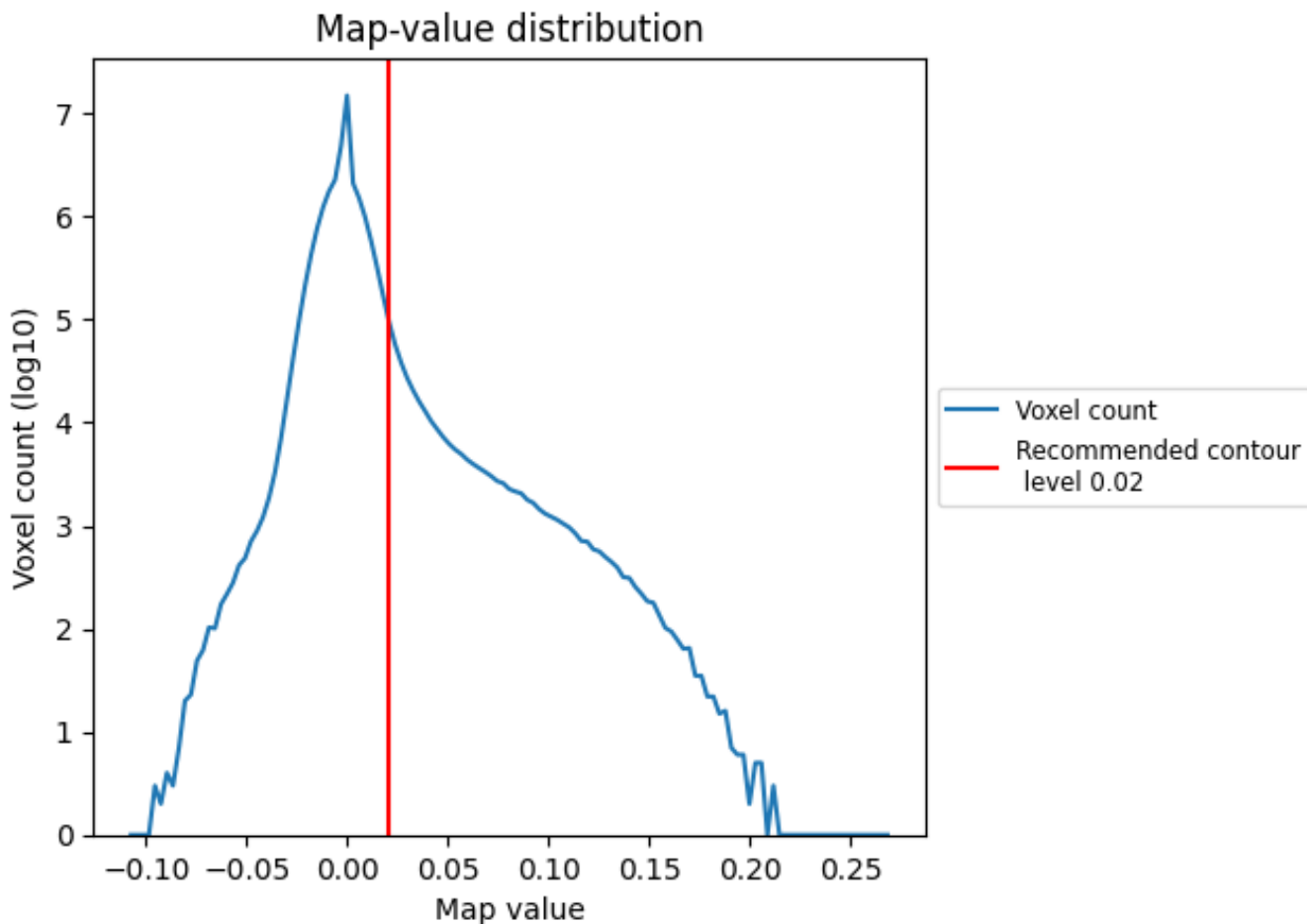
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

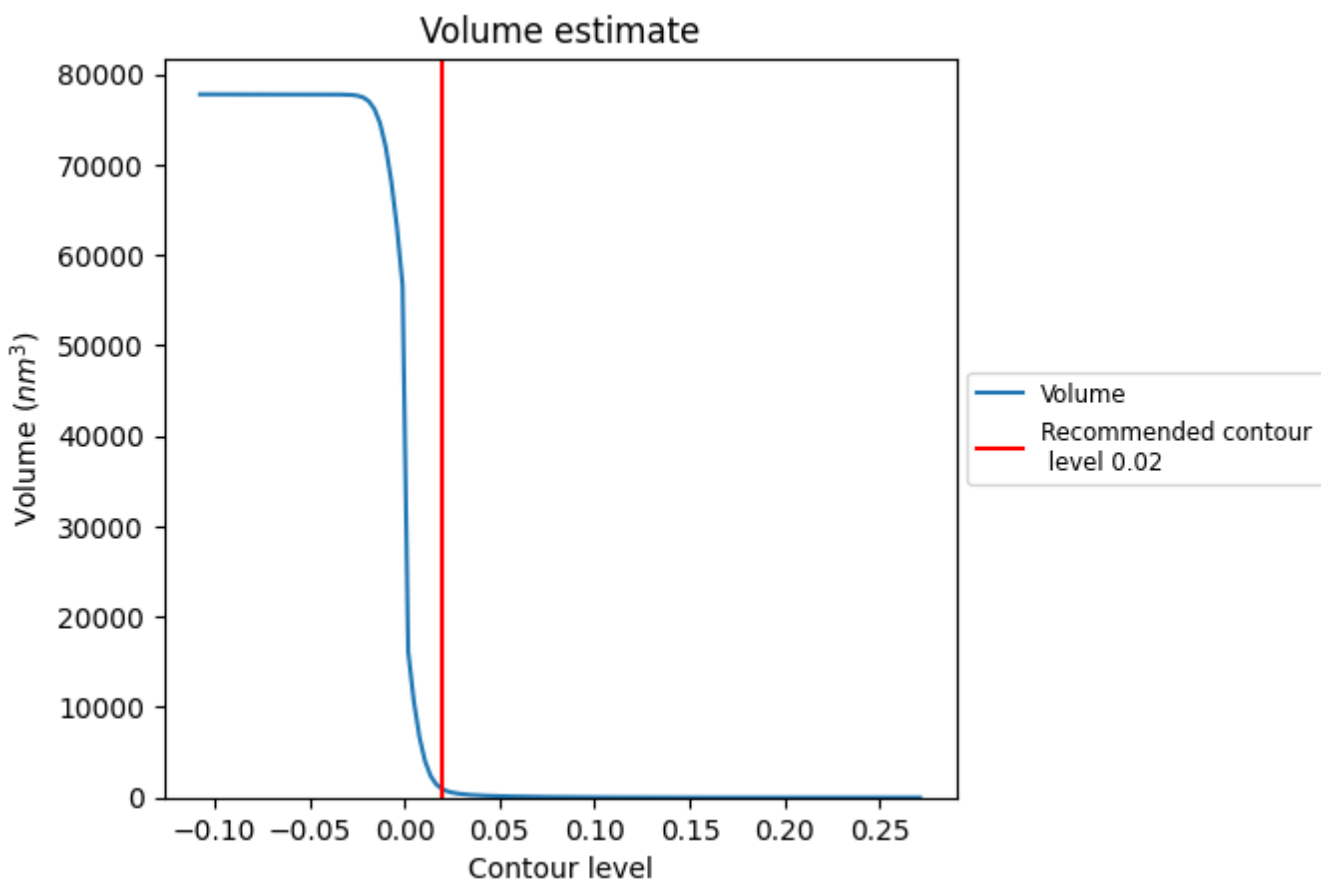
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

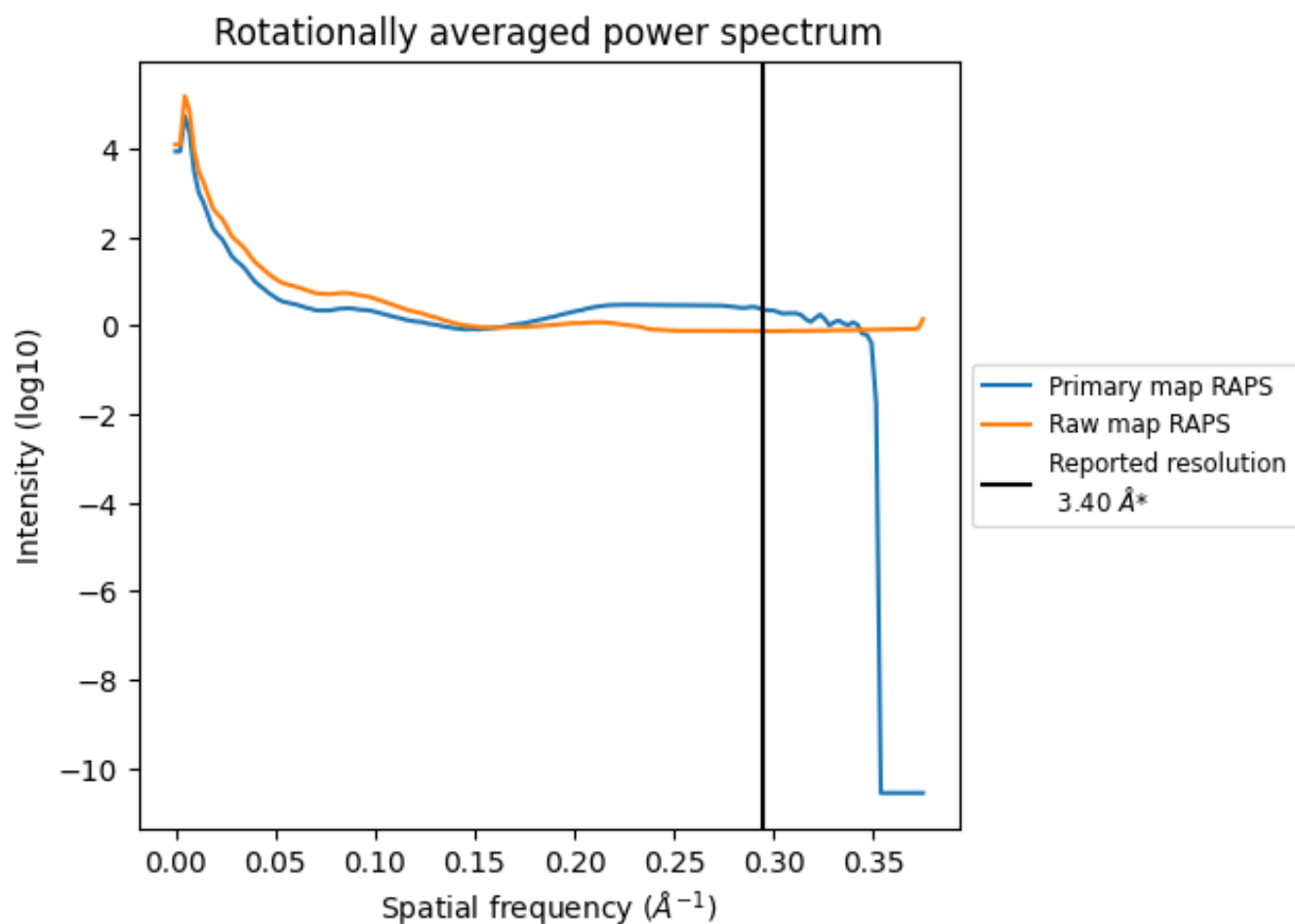
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 931 nm³; this corresponds to an approximate mass of 841 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

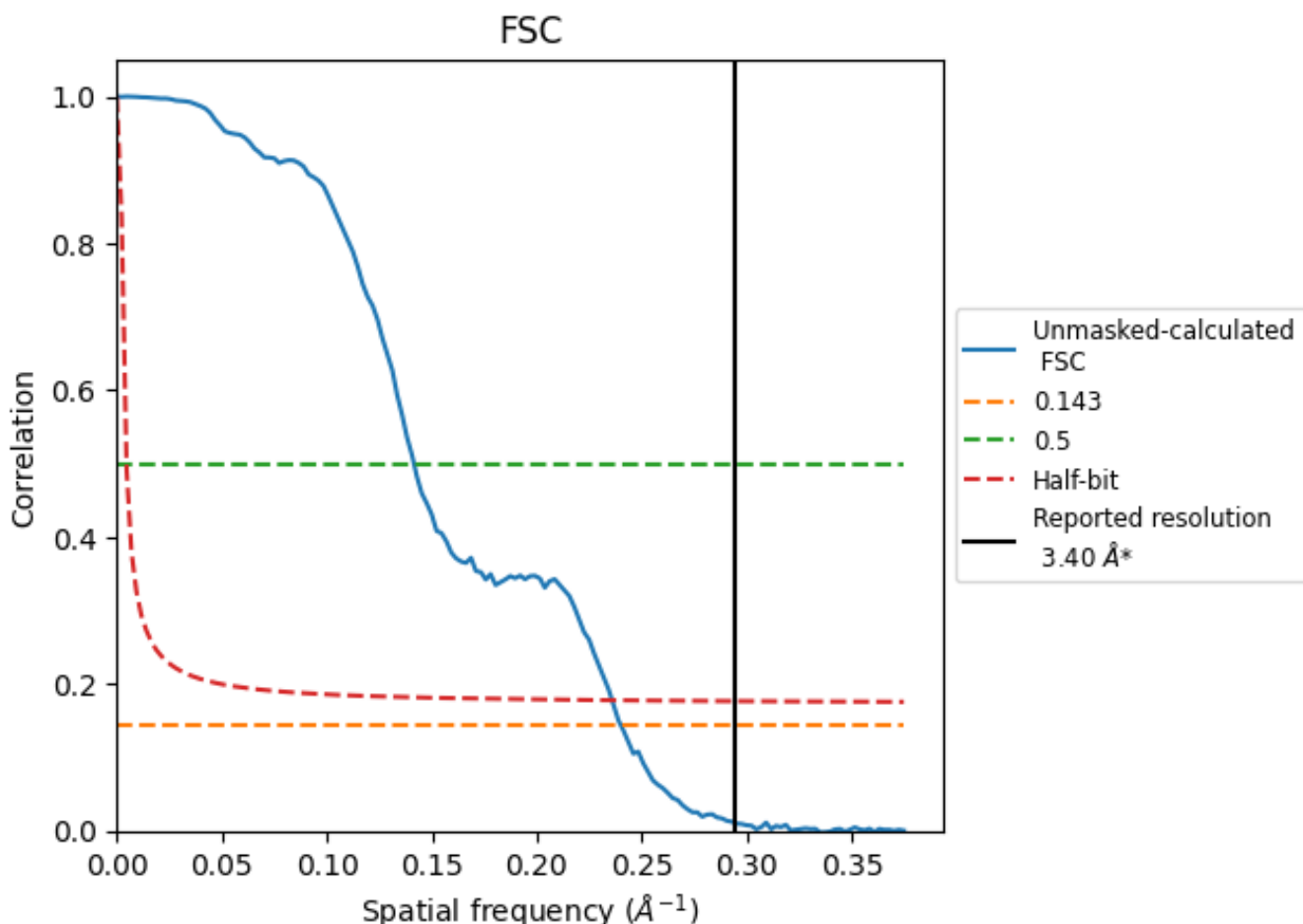


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

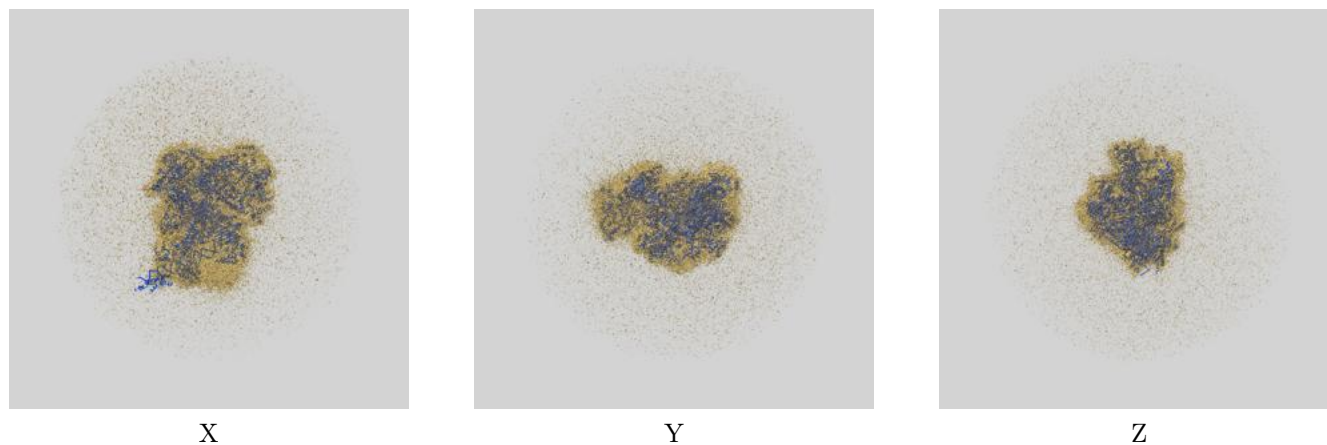
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.16	7.07	4.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.16 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

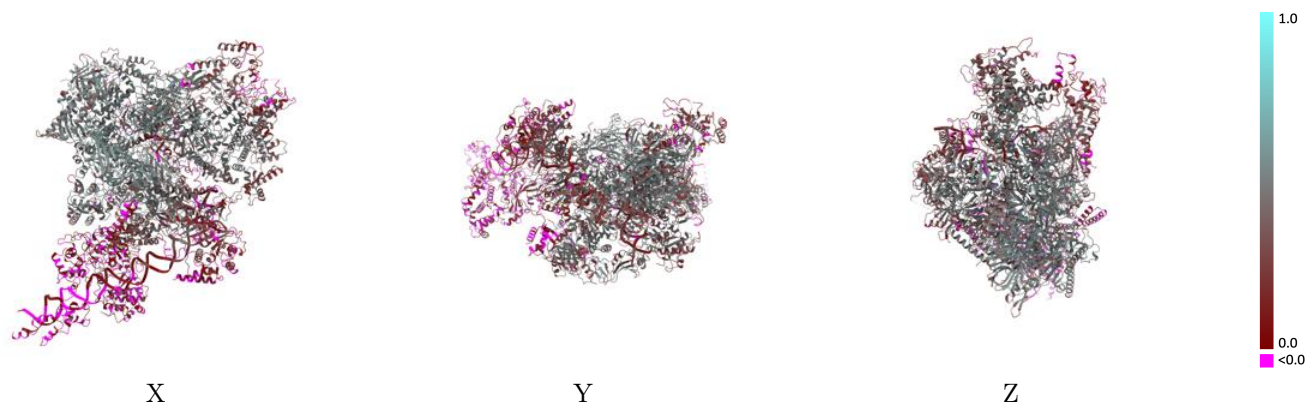
This section contains information regarding the fit between EMDB map EMD-35722 and PDB model 8IUH. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



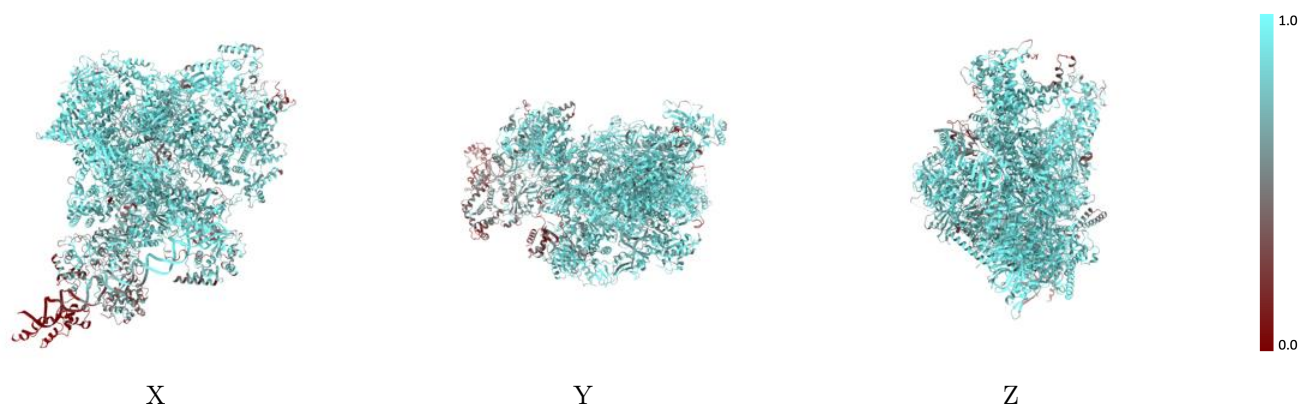
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [\(i\)](#)



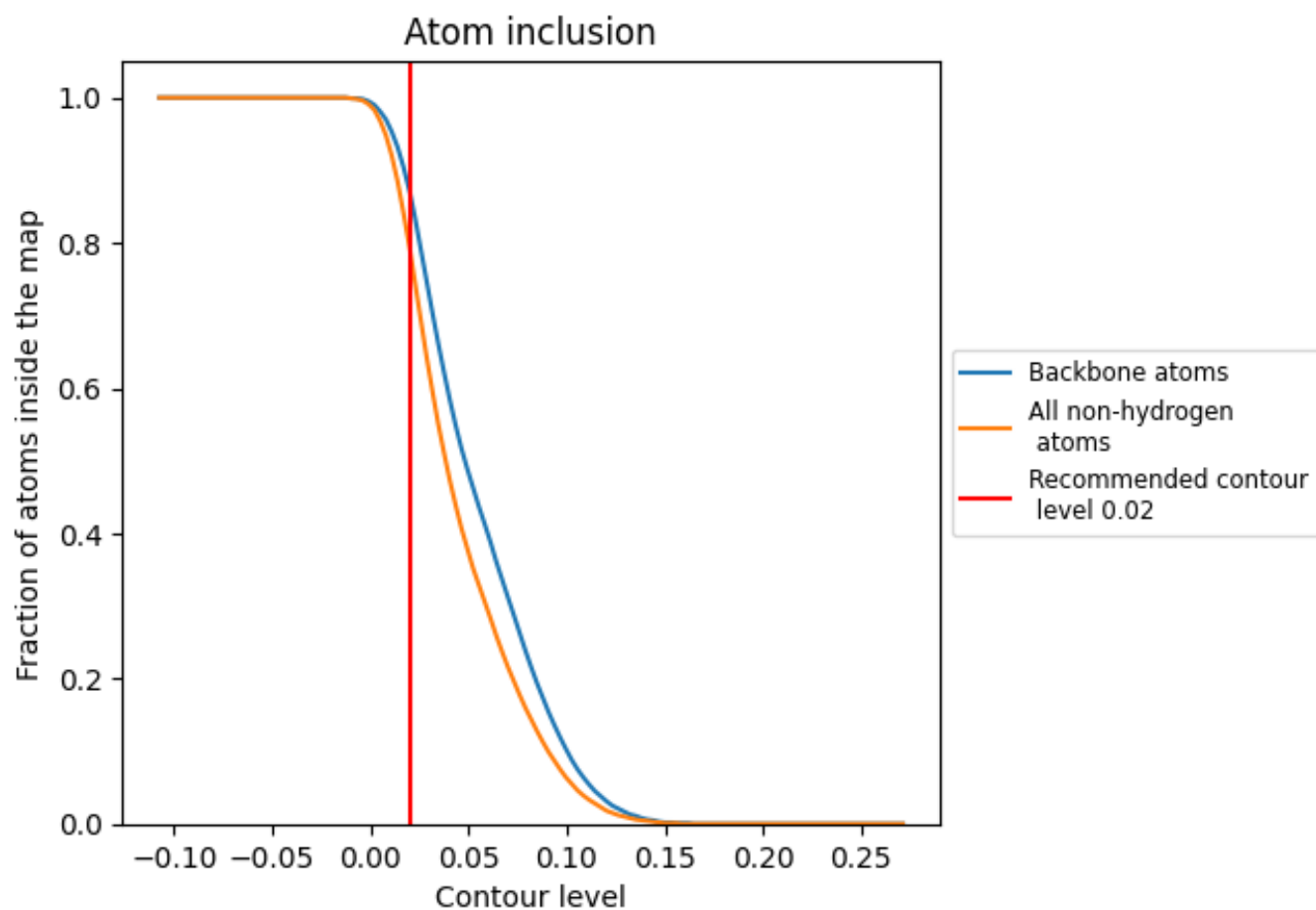
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).





















































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7920	 0.3410
1	 0.4990	 0.0360
3	 0.5890	 0.1040
4	 0.4030	 0.0500
A	 0.8950	 0.4600
B	 0.9140	 0.4830
C	 0.9040	 0.4850
D	 0.7710	 0.2470
E	 0.8480	 0.3780
F	 0.9270	 0.4910
G	 0.8450	 0.3380
H	 0.8590	 0.4510
I	 0.6760	 0.2470
J	 0.9340	 0.5060
K	 0.8920	 0.4660
L	 0.8840	 0.4070
M	 0.8080	 0.3730
N	 0.7700	 0.3590
O	 0.8160	 0.3640
P	 0.6880	 0.2380
Q	 0.7570	 0.2920
U	 0.8210	 0.2440
V	 0.7790	 0.2980
W	 0.6760	 0.1300
X	 0.6490	 0.1050
Y	 0.6490	 0.1450

